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Vincent Rat, Pascal André, Jacques Aubreton, Marie-Françoise Elchinger, Pierre Fauchais, André Lefort

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V. Rat[1], P. André[2], J. Aubreton[1], M.F. Elchinger[1], P. Fauchais[1], and A. Lefort[2]

[1] *SPCTS University of Limoges, 123 av. A. Thomas, 87060 Limoges cedex, France*
[2] *LAEPT Blaise Pascal University, 24 av. des Landais, 63177 Aubière cedex, France*

Abstract

A new derivation of transport properties in a two-temperature plasma has been performed. The electron kinetic temperature T_e is supposed to be different from that of heavy species T_h. The resolution of the Boltzmann's equation, thanks to the Chapman-Enskog method, is used to calculate transport coefficients and it allows to the generalisation of bracket integrals out of thermal equilibrium. Two-temperature diffusion coefficients are defined and the obtained results are presented for an atmospheric two-temperature argon plasma.

1. Introduction

Recent works [1] have shown that the simplified theory of transport properties out of thermal equilibrium introduced by Devoto [2] and Bonnefoi [3] neglecting the coupling between electrons and heavy species, and very often used in modeling, leads to unphysical results. Thus, two-temperature transport coefficients have been derived [4] without the Bonnefoi's assumptions starting from the Boltzmann's equation. The electron temperature T_e is supposed to be different from that of heavy species T_h. Only elastic processes are considered in a collision dominated plasma. Firstly, is presented the principle of the resolution of the Boltzmann's equation in a two-temperature model. Secondly, the modifications of this resolution, with respect to equilibrium, give rise to a generalisation of bracket integrals giving transport coefficients. The differences with thermal equilibrium are then highlighted. Lastly, two-temperature diffusion coefficients resulting of this derivation are displayed as function of the non-equilibruim parameter $\theta = T_e / T_h$.

2. Resolution of the Boltzmann equation

The distribution function f_i of the ith species is the solution of the integro-differential equation of Boltzmann [5]:

$$\frac{Df_i}{Dt} = \sum_{j=1}^{N} \iiint \left(f'_i f'_j - f_i f_j \right) g b\, db\, d\varepsilon\, d\vec{v}_j \quad , \qquad (1)$$

f'_i is the distribution function after the elastic collision of the ith species, g is the relative velocity of the species i and j, b and ε are respectively the impact parameter and the incidence azimuthal angle.

It has been assumed that the zero-order approximation function is Maxwellian at T_e for electrons and T_h for heavy species. The distribution function of the ith species, solution of (1), is approximated by a Maxwellian distribution function $f_i^{(0)}$ perturbed by a slowly time and space dependent first-order perturbation function Φ_i of the ith species with the temperature T_i:

$$f_i = f_i^{(0)}(1+\Phi_i) \tag{2}$$

Inserting (2) into (1), it can be shown that:

$$\frac{Df_i^{(0)}}{Dt} = I_i^{(0)} + \sum_{j=1}^{N} \iiint f_i^{(0)} f_j^{(0)} \left((\Phi'_i + \Phi'_j) K_i - \Phi_i - \Phi_j \right) g b\, db\, d\varepsilon\, d\vec{v}_j \tag{3}$$

$I_i^{(0)}$ represents the zero-order approximation of the Chapman-Enskog's expansion and does not vanish for two colliding particles with different temperatures:

$$I_i^{(0)} = \sum_{j=1}^{N} \iiint \left(f'^{(0)}_i f'^{(0)}_j - f_i^{(0)} f_j^{(0)} \right) g b\, db\, d\varepsilon\, d\vec{v}_j \tag{4}$$

A term $K_i(W_i, \theta_{ij})$, taking into account the thermal non-equilibrium when electrons and heavy species collide, has been introduced as follows:

$$f'^{(0)}_i f'^{(0)}_j = f_i^{(0)} f_j^{(0)} K_i(W_i, \theta_{ij}) \qquad \forall i, j \in [1; N] \tag{5}$$

where $$K_i(W_i, \theta_{ij}) = \exp\left(-\left(W'^2_i - W_i^2\right)(1-\theta_{ij})\right) \tag{6}$$

with $$\theta_{ij} = \frac{T_i}{T_j} \tag{7}$$

and W'_i is the reduced velocity after collision such as $\vec{W}_i = \left(\frac{m_i}{2kT_i}\right)^{\frac{1}{2}} \vec{V}_i$ where $\vec{V}_i = \vec{v}_i - \vec{v}_0$. $\vec{v}_i$ and $\vec{v}_0$ are respectively the velocity of the ith species and flow velocity. The introduction of K_i allows the definition of bracket integrals to be generalised out of thermal equilibrium.

The calculation of $\frac{Df_1^{(0)}}{Dt}$ and $\frac{Df_i^{(0)}}{Dt}$ $(i \geq 2)$ is obtained using the equations of change [4]. The transport terms in equations (3), show that transport phenomena are due to a new gradient $\vec{\nabla} \ln \theta$, which characterizes the temperature difference between electrons and heavy species, the heavy species temperature gradient, the velocity gradient, external forces (forced diffusion), the concentration and pressure gradients and a term acting on the hydrostatic pressure to the first-order approximation of Sonine polynomials.

Following the linear form of transport terms, it can be supposed that the first-order perturbation function can be written as:

$$\Phi_i = -\vec{A}_i . \vec{\nabla}\ln T_h - \vec{B}_i : \vec{\nabla}\vec{v}_0 + \sum_{j=1}^{N} \vec{C}_i^j . \vec{d}_j + D_i Q_1^{(0)} + \sum_{j=1}^{N} \vec{E}_i^j . g_j \vec{\nabla}\ln\theta - \vec{F}_i . \vec{\nabla}\ln\theta \quad (8)$$

The diffusion forces are written as follows for *electrons*:

$$\vec{d}_1 = \frac{\rho_1}{\rho} \sum_{j=1}^{N} n_j \vec{F}_j - n_1 \vec{F}_1 + \left(\frac{x_1 \theta}{D} - \frac{\rho_1}{\rho} \right) \vec{\nabla} p + \frac{\theta p}{D^2} \vec{\nabla} x_1 \quad (9)$$

and $$g_1 = \frac{x_1 p (1 - x_1)}{D^2} \quad (10)$$

For *heavy species*, it is written:

$$\vec{d}_i = \frac{\rho_i}{\rho} \sum_{j=1}^{N} n_j \vec{F}_j - n_i \vec{F}_i + \left(\frac{x_i}{D} - \frac{\rho_i}{\rho} \right) \vec{\nabla} p + \frac{p}{D} \vec{\nabla} x_i - \frac{x_i (\theta - 1) p}{D^2} \vec{\nabla} x_1 \quad (11)$$

and $$g_i = -\frac{x_i x_1 p}{D^2} \quad (12)$$

ρ_i, $\vec{F}_i$, x_i and p are respectively the density, an external force and the molar fraction of the ith species and the total pressure.
$Q_1^{(0)}$ corresponds to the exchanged kinetic energy between electrons and heavy species during collisions. It can be shown:

$$Q_1^{(0)} = 4 k_B n_1 (T_h - T_e) \left(\frac{8 k_B T_e}{\pi m_1} \right)^{\frac{1}{2}} \sum_{j=2}^{N} n_j \frac{m_1}{m_j} \overline{Q}_{1j}^{(1,1)} \quad (13)$$

k_B being the Boltzmann constant.
The unknowns $\vec{A}_i$, $\vec{B}_i$, $\vec{C}_i^j$, D_i, $\vec{E}_i^j$ and $\vec{F}_i$ are determined by assuming that they can be splitted on the Sonine polynomial basis [5] which allows the introduction of systems of linear equations following the approximation order.
The introduction of $\vec{\nabla}\ln\theta$ prevents from considering the uncoupling between electrons and heavy species in the resolution of systems of linear equations which gives the transport coefficients. As a result, two-temperature diffusion coefficients not only include ordinary and thermal diffusion but also new diffusion coefficients due to the temperature difference ($\vec{\nabla}\ln\theta$) between electrons and heavy species [4].

3. Bracket integrals

Transport coefficients results in the resolution of systems of linear equations. Each element q_{ij}^{mp} (m and p represents the order of approximation of Sonine polynomials) of the considered matrix depends on bracket integrals. The latter are expressed as a linear combination of collision integrals which account for the interaction between the colliding species.
For example, in the first-order approximation of Sonine polynomials, the following bracket integral can be written:

$$\left[\vec{W}_i S^1_{\frac{3}{2}} \left(W_i^2 \right), \vec{W}_j S^1_{\frac{3}{2}} \left(W_j^2 \right) \right]_{ij} = C \sum_{r\ell} A_{11r\ell} \Omega_{ij}^{(r,\ell)} \quad (14)$$

where C depends on m_i, m_j, T_i and T_j.

$\Omega_{ij}^{(r,\ell)}$, i and j being the colliding species, is the integral of the transport cross section over a Maxwellian distribution function. Table 1 gives the values of the coefficients $A_{11r\ell}$ at equilibrium ($\theta = 1.0$) and for different values of θ calculated for a collision between an electron and a heavy species, that is for a mass ratio of 10^{-5}.

Table I: Calculation of $A_{11r\ell}$ for different values of θ and with a mass ratio $m_j/m_i = 10^{-5}$.

θ	1.00	1.25	1.50	2.00	3.00
A_{1111}	-13.75	-8.50	-5.00	-0.63	-3.75
A_{1121}	5.00	3.30	3.00	4.50	11.00
A_{1122}	2.00	0.75	-0.50	-3.00	-8.00
A_{1131}	-1.00	-1.40	-2.00	-3.50	-7.00
A_{1132}	0.00	0.50	1.00	2.00	4.00

Firstly, it is shown that our results strictly lead to those of Hirschfelder et al [5]. Secondly, the coefficients $A_{11r\ell}$ are drastically changed following the applied thermal non-equilibrium. Lastly, coefficients such as A_{1132} do not vanish when the non-equilibrium parameter θ is different from unity. As a result, collision integrals $\Omega_{ij}^{(r,\ell)}$ with indexes (r,ℓ) higher than at thermal equilibrium should be taken into account out of thermal equilibrium.

4. Two-temperature diffusion coefficients

Two-temperature diffusion coefficients are displayed for a two-temperature argon plasma. Calculations are performed at atmospheric pressure and the two-temperature plasma composition is obtained using the Saha equation for ionization of Van de Sanden et al [6]. Electrons, Ar and Ar^+ species have been considered.

First, it has to be noted that the rate of convergence of diffusion coefficients are similar to that of thermal equilibrium that is the second-order approximation is sufficient for diffusion coefficients implying electrons. However, for argon, around 5000 K (the electron temperature) the third-order approximation is required because of the Ramsauer effect of the momentum cross section.

The two-temperature diffusion coefficients D_{eAr} and D_{Ar^+e} are respectively displayed in figure 1(a) and 1(b) as a function the electron temperature from 1000 up to 20000 for different values of θ (between 1 and 3). The calculation have been performed to the third-order approximation. When ionisation is weak, namely below 6000 K, two-temperature ordinary diffusion coefficients increase with temperature.

For D_{eAr}, the effect of temperature is dominant with respect to the collision integral $\overline{Q}_{eAr}^{(1,1)}$ which increases slowly with T_e. However, between 4500 and about 6000 K, the effect of the collision integral $\overline{Q}_{eAr}^{(1,1)}$ overcomes the effect of temperature but, at these temperatures the binary approximation is not valid anymore. As a result, the Ar^+ species has to be taken into account and the effect of the charge transfer collision integral $\overline{Q}_{ArAr^+}^{(1,1)}$ contributes to increase ordinary diffusion coefficients since it decreases with temperature faster than $\overline{Q}^{(1,1)}_{eAr}$ increases (for example, $\overline{Q}^{(1,1)}_{ArAr^+} / \overline{Q}^{(1,1)}_{eAr}$ is about 55 at 5000 K). The same evolution for D_{Ar^+e} is observed, the charge transfer collision integral being dominant at low temperature.

When ionization becomes significant around 6000 K, D_{eAr} and D_{Ar^+e} decreases with temperature because the charged-charged collision integral $\overline{Q}^{(1,1)}_{eAr^+}$ counterbalances the effect of temperature.

Besides, it is observed in figure 1(a) and 1(b) that two-temperature diffusion coefficients decrease with the non-equilibrium parameter θ. Figure 2 depicts the influence of the non equilibrium parameter θ on diffusion coefficients and that it can be writen that at low temperature $D_{eAr} = \theta D_{Are}$.

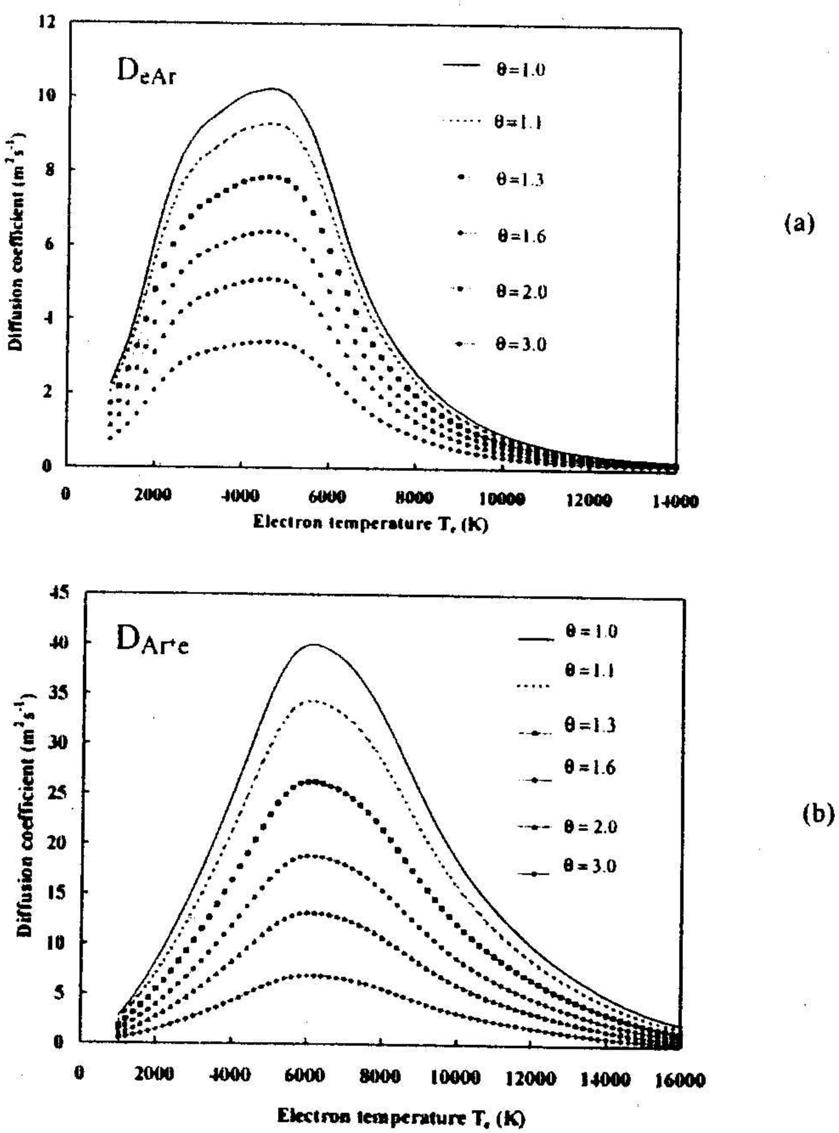

Figure 1: Two-temperature diffusion coefficient D_{eAr} (a) and D_{Ar^+e} (b) as function of electron temperature T_e and θ.

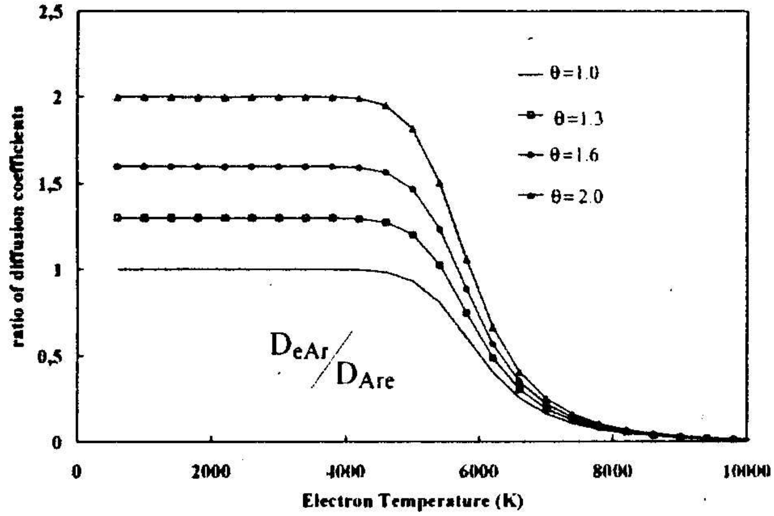

Figure 2: Ratio D_{eAr}/D_{Are} as function of electron temperature T_e and θ.

5. Conclusion

A new method of derivation of transport properties in a two-temperature plasma has been performed. Two-temperature transport coefficients have been derived starting from the Boltzmann's equation. The latter is solved by using the well-known Chapman-Enskog method which has been adapted to thermal non-equilibrium plasmas. It has been assumed that the distribution function of species, solution of the Boltzmann's equation, is a Maxwellian, at T_e for electrons and T_h for heavy species, perturbed by a slowly time and space dependent first-order perturbation function. The introduction of the gradient $\vec{\nabla}\theta$ allows to maintain the coupling between electrons and heavy species in the calculation of two-temperature transport coefficients. Two-temperature diffusion coefficients in an atmospheric argon plasma were calculated between electrons and heavy species, contrarily to what happens when using the simplified theory of transport coefficients of Devoto[2] and Bonnefoi [3].

References

[1] V. Rat, J. Aubreton, M.F. Elchinger, and P. Fauchais, Plasma Chem. Plasma Process. **21** (2001),.355-364.
[2] R.S. Devoto, Phys. Fluids **10** (1967), 2105-2112.
[3] C. Bonnefoi, State Thesis, University of Limoges, France (1983).
[4] V.Rat, P. André, J. Aubreton, M.F. Elchinger, P. Fauchais, and A. Lefort, to be published, Phys. Rev. E.
[5] J.O. Hirschfelder, C.F. Curtis, and R.B. Bird, Molecular Theory of Gases and Liquids, 2nd ed., Wiley, New York (1964).
[6] M.C.M. Van de Sanden, P.P.J.M. Schram, A.G. Peeters, J.A.M. van der Mullen and G.M. Kroesen, *Physical Review A*, **40** (1989), 5273-5276.